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Theoretical investigations of defects in a Si-based digital ferromagnetic heterostructure – a spintronic material

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We investigate the effects of two different forms of defects on the half-metallic properties of the Mn/Si digital ferromagnetic heterostructure (DFH) (PRL **96**,027211 (2006)) using a first principles algorithm based on density functional theory. The half metallicity is retained when the δ-layer of the Mn atoms has 25% imperfection including a vacancy. The crucial properties of the DFH are robust against 25% defects.

1 INTRODUCTION

Spintronics[1] is a new operational paradigm in semiconductor technologies wherein the electron's spin is utilized in addition to its charge. Among spintronic materials half metals are extremely attractive because, according to the Julliere[2] formula, they are expected to show infinite magnetoresistance. A half metal has one spin states exhibiting metallic behavior while the other channel shows semiconducting properties. Therefore, it has 100% spin polarization of the carriers at the Fermi energy, E_F. Theoretically, several groups including our own using spin-polarized first-principles algorithms[3] with the generalized gradient approximation (GGA)[4] have predicted half metallic transition metal pnictides[5,6], carbides[7,8], chacogenides[9], a superlattice[10] and a quantum dot[11], each with the zinc-blende (ZB) structure. Sanvito and Hill[12] examined a δ-layer of Mn in GaAs, a digital ferromagnetic heterostructure (DFH), exhibiting two dimensional half-metallic features. However, due to the difficulties in growth of half metallic materials with the ZB structure, the actual fabrication of any devices has yet to be realized.

Among the semiconductor industries, Si related technologies are farther advanced than other semiconductors with respect to growth and nanofabrication. To take advantage of these advances it is necessary to find Si-based spintronic materials, and in particular those exhibiting half-metallic properties. Recently, we proposed a Si-based DFH, Mn/Si DFH.[13] It not only exhibits two dimensional half metallic properties but also can avoid the possibility of a T* at which the half-metallicity disappears, such as in the Heusler alloys due to spin flip transitions.[14] However, our proposed Mn/Si DFH[13] has an ideal δ-layer of Mn atoms. Since it is essentially impossible to grow such an ideal structure, we address the issue of how defects affect the two-dimensional half metallicity in the Mn/Si DFH. In this paper, we report on investigations of Si based DFHs having imperfections in the δ-layer of Mn. Two cases have been examined: the δ-layer with up to (i) a 25% imperfection but without any vacancy, and (ii) 25% vacancy in the δ-layer.

2. BRIEF DISCUSSION OF CALCULATIONAL METHOD AND MODELS

We used the well-documented spin-polarized VASP code[3] with the GGA[4] to treat the electron-electron correlations. The ultra-soft pseudopotentials[15] for Si and Mn are generated under the normal valence electronic configurations of the atoms. Plane waves are used as the basis functions.

In Ref. 13, the 32–atom model is too small to simulate any defects (one Mn atom/unit-cell) in the δ-layer. By expanding the lattice constants along the **x** and **y**-directions of the 32-atom model a factor two each to accommodate four Mn atoms in a layer, the lattice constants along the two directions now are $\sqrt{2}$ a, where a is the lattice constant of the conventional cubic cell. In the **z**-direction, the model has 16 layers instead of 32 layers as in Ref. 13. The new supercell consists of 64 atoms and is shown in Fig 1(a) including the atoms at the cell boundaries to show the periodicity. Mn atoms are shown in red and the blue circles are the Si atoms. This model defines the 64-atom supercell. The models having defects are modified from this one (Fig. 1(a)).

With the models defined, we use the E_{cut} of 650 eV to determine the number of plane waves. The results of the 64-atom model, with the Monkhorst-Pack[16] mesh of (11,11,1) agree with the (15,15,1) used in Ref. 13. For the defect cases, we used (11,11,3) to generate the special **k**-points for constructing the charge density for more localized states associated with defects. The total energy of each model is converged to better than 1.0 meV. All the atoms except at the origin of the unit cell are relaxed such that the components of any force acting on an atom are less than or equal to 6.0 meV/Å.

3. RESULS AND DISCUSSION

3.1 Comparison of the 64-atom and the 32-atom supercells: The 64-atom supercell for the ideal Mn/Si DFH shown in Fig. 1(a) will serve as a reference for studying the defects. To make sure that this model gives identical results of the 32-atom supercell, we optimized the lattice constant of this large cell. It shows only a small increase (0.02 Å). Since the ferromagnetic phase in the DFH has been shown to have the lower total energy from the earlier study[13], here we omit treatment of the anti-ferromagnetic case. The up spin channel shows metallic properties while the down spin states exhibit semiconducting behavior agreeing with the results of Ref. 13. In Table I, we summarize the comparison of the optimized lattice constants, the semiconducting gap energy, and the magnetic moment/unit-cell.

Table I. Summary of the optimized lattice constant, the gap energy (eV) in the semiconducting channel, and the magnetic moment (μ_B/cell) between the 32- and 64-atom supercells and the gap energy in the relaxed models. Energy is in eV.

Case	Optimized lattice constant (Å)	Gap energy (eV)	Magnetic moment (μ_B/cell)
32-atom	5.45	0.25	12.00
64-atom	5.47	0.25	12.00

We emphasize that an integer value of the magnetic moment/unit-cell is a necessary condition for a sample to be a half-metal, in particular for theoretical predications. The reason is that the total number of electrons in a unit cell is an integer. In the semiconducting channel, the number of electrons filling up to the top of the valence band is also an integer. Consequently, the number of electrons in the conducting states is also an integer. The listed magnetic moment can be accounted for by the so-called ionic model discussed in Ref. 17. Each Mn is surrounded by four Si. They take four electrons away from the Mn atom to form the d-p hybridized bonds. The three electrons remaining at the Mn align their spins. With the g-factor of 2, the resultant moment at each Mn is 3.0 μ_B. There are four Mn atoms in the unit cell, so the moment is 12.00 μ_B/cell.

3.2 Defect cases We consider two defects: (i) one Mn atom in the δ-layer is replaced by a Si atom representing 25% imperfection, and (ii) a vacancy in the δ-layer made by removing a Mn atom.

3.2.1 Configuration (i) The relaxed 64-atom model with one Mn atom replaced by a Si atom is shown in (Fig. 1(b)). The total energy of this defect case is higher than the case of the perfect δ-layer by 12.98 eV. This energy value involves the chemical potential difference of the Mn and the Si atoms. The electronic properties of this relaxed defect model show half metallic properties. The minority spin channel exhibits a gap of 0.29 eV. The magnetic moment is 9.0 μ_B/cell.

3.2.2 Configuration (ii) In this configuration, the defect in the δ-layer is a vacancy. The relaxed model is shown in Fig. 1(c). The vacancy is presented in the middle (missing between two red atoms shown in the layer due to periodicity). The electronic properties of this model also show half metallic properties. The minority spin channel exhibits a gap of 0.32 eV and the magnetic moment is 9.0.

Table II. Comparison of the gap energy, and the magnetic moments for the perfect δ-layer and the two defect cases.

Case	Gap energy (eV)	Magnetic Moment (μ_B/unit-cell)
Relaxed ideal DFH	0.25	12.0
Case (i)	0.26	9.0

Case (ii)	0.32	9.0

4. Summary

In summary, we investigate two kinds of defects in a Si-based DFH with Mn as the transition metal element. A 64-atom supercell with four Mn atoms in the δ-layer and 15 layers of Si is used to model the DFH having a defect. We first check the properties of this larger supercell against the ones reported in Ref. 13. The gap in the minority channel is 0.25 eV and the magnetic moment of 12.00 μ_B/unit-cell agree well with the earlier 32-atom supercell.[13]

In the two defect cases, each preserves the two-dimensional half metallic behavior (confirmed also by densities of states, not shown). We therefore suggest that it is worthwhile to try growing DFHs using the molecular beam epitaxial method because a perfect δ-layer is not required.

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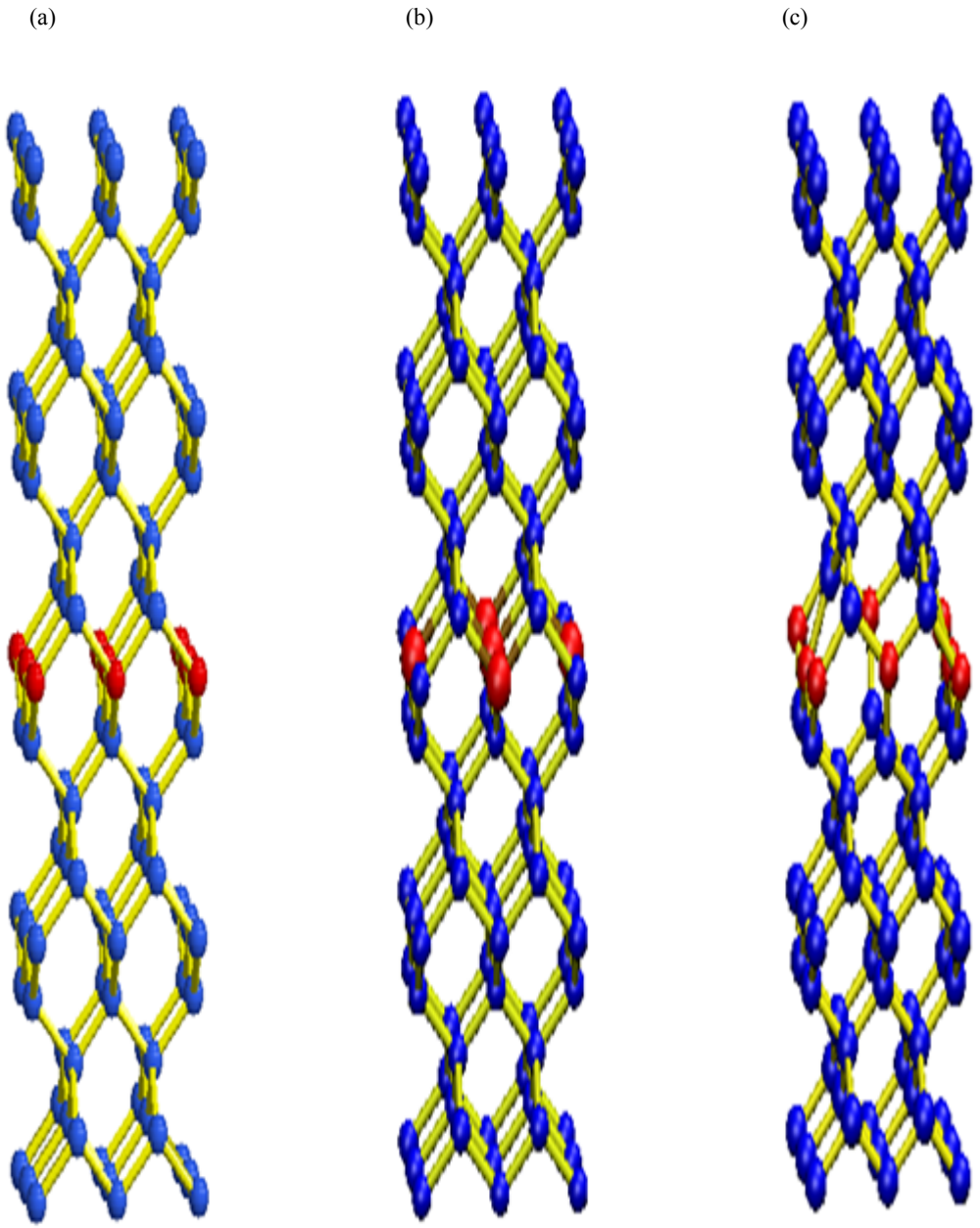

Fig. 1. (a) The 64-atom supercell model having the perfect δ-layer serving as a reference. The red spheres are the Mn atoms. The blue spheres are the Si atoms. (b) with a Mn substituted by a Si - model having 25% defect without a vacancy.